International Journal of Quantum Chemistry Author Index—Volume 57

Ågren, H. See Minaev, B. F., 519

Aida, M.

—; Kaneko, M.; Dupuis, M.: An Ab Initio MO Study on the Thymine Dimer and Its Radical Cation, 949

Alacid, M. See Zúñiga, J., 43

Alkorta, I.

—; Perez, J. J.: Molecular Polarization Potential Maps of the Nucleic Acid Bases, 123

Altmann, J. A.

—; Handy, N. C.; Ingamells, V. E.: A Study of the Performance of Numerical Basis Sets in DFT Calculations on Sulfur-Containing Molecules, 533

André, J.-M. See Champagne, B., 811

André, J. M. See Flamant, I., 871

Andreev, Ye. A.

—; Repyakh, I. V.: Quantum Chemical Study of Self-Organized Water Fractals, 767

Andrés, J. See Cárdenas, R., 245

Andrés, J. See Martins, J. B. L., 861

Antonsen, F. See Avery, J., 401

Aray, Y. See Keith, T. A., 183

Avery, J.

—; Hansen, T. B.; Wang, M.; Antonsen, F.: Sturmian Basis Sets in Momentum Space, 401

Bacchus-Montabonel, M. C.

—; Fraija, F.: State-Selective Electron Capture Processes in Collisions Involving Boron Ions, 611

Bader, R. F. W. See Keith, T. A., 183

Baerends, E. J. See Gritsenko, O., 17

Baerends, E. J. See van Lenthe, E., 281

Barone, G. See La Manna, G., 971

Bastida, A. See Zúñiga, J., 43

Berendsen, H. J. C.

—; Mavri, J.: Approach to Nonadiabatic Transitions by Density Matrix Evolution and Molecular Dynamics Simulations, 975

Berrondo, M.

—; Rivas-Silva, J. F.: Cluster Models of Ionic Crystals: Band Gaps, 1115

Bianchi, R.

—; Bressanini, D.; Cremaschi, P.; Mella, M.; Morosi, G.: Wave-Function Optimization by Least-Squares Fitting of the Exact Wave Function Sampled by Quantum Monte Carlo, 321

Bishop, R. F.

—; Hale, R. G.; Xian, Y.: A Microscopic Study of the quantum Critical Behavior of the Spin-$\frac{1}{2}$ Anisotropic Heisenberg Models, 919

Boča, R.

Platinum-Centered Octakis (Triphenylphosphino gold) Cluseters: A Relativistic MO Study, 735

Bonapasta, A. A.

—; Pavesi, L.: Hydrogen Interaction with Shallow and Deep Centers in GaAs, 823

Bouferguene, A.

—; Fares, M.; Hoggan, P. E.: STOP: A Slater-Type Orbital Package for Molecular Electronic Structure Determination, 801

Bracken, P.

Investigation of Some Soluble Lattice Spin Models, 235

Bracken, P.

—; Čížek, J.: Interpolant Polynomial Technique Applied to the PPP Model. I. Asymptotics for Excited States of Cyclic Polyenes in the Finite Cyclic Hubbard Model, 1019

Bracken, P. See Čížek, J., 1033

Brändas, E. J.

Review of *Algebraic Approach to Simple Quantum Systems*, by Barry G. Adams, 259

Brändas, E. J.

Review of *The Beginnings of Cancer in the Cell*, by Janos Ladik and Wolfgang Förner, 261

Breitkopf, C. See Friedemann, R., 943

Bressanini, D. See Bianchi, R., 321

Bu, Y.

—; Cao, Z.; Song, X.: Ab Initio Studies on Hydrogen-Transfer Tunneling for Cl + HCl Abstraction Hydrogen Reaction, 95

Burke, K. See Perdew, J. P., 309

Campillo, M. See Cárdenas, R., 245

Cao, Z. See Bu, Y., 95

Cárdenas, R.

—; Andrés, J.; Krechl, J.; Campillo, M.; Tapia, O.: On a Possible Invariance of a Transition Structure to the Effects Produced by Ancillary H-Bonding Molecules: Modeling the Effects of Ser-48 in the Hydride-Transfer Step of Liver Alcohol Dehydrogenase, 245

Castellani, N. J. See Mikušík, P., 887

Champagne, B.
—; André, J.-M.; Öhrn, Y.: Ab Initio Dynamic Polarizabilities of Polymers. I. Hydrogen Chain Models, 811
Chang, T.-C. See Ho, T.-M., 229
Cheng, V. K. W.
—; Flock, M.; Ramek, M.: Ab Initio SCF Structure Investigation of β-Hydroxypropionic Acid and 3-Aminopropionamide, 929
Čížek, J.
—; Bracken, P.: Interpolant Polynomial Technique Applied to the PPP Model. II. Testing the Interpolant Technique on the Hubbard Model, 1033
Čížek, J. See Bracken, P., 1019
Colombo, S. See Gianinetti, E., 369
Cooper, D. L.
—; Ponec, R.; Thorsteinsson, T.; Raos, G.: Pair Populations and Effective Valencies from AB Initio SCF and Spin-Coupled Wave Functions, 501
Cremaschi, P. See Bianchi, R., 321
Cremer, D. See He, Z., 157
Csavinszky, P.
Numerical Investigation of a Lower Bound to the Thomas–Fermi Kinetic Energy and the Validity of the Lieb Conjecture for H^-, He, Li^-, B^{3+}, O^{6+}, Ne^{8+}, and Mg^{12+}, 449

Daniel, C.
—; Vivie-Riedle, R. De.; Heitz, M.-C.; Manz, J.; Saalfrank, P.: From Laser Control of Vibrationally Mediated Photodissociation to Photodesorption: Model Simulations of Breaking Metal–Ligand Bonds in Organometallic Molecules, Clusters, and Adsorbates at Surfaces, 595
Darkhovsky, M. B. See Tchougréeff, A. L., 903
Datta, S. N. See Trindle, C., 781
Day Jr., O. W.
The Extended Koopmans' Theorem Fock Operator and the Generalized Overlap Amplitude One-Electron Operator, 391
Day Jr., O. W. See Morrison, R. C., 355
Delhalle, J. See Flamant, I., 871
Demangeat, C. See Mikušík, P., 887
de Vries, A. H.
—; van Duijnen, P. Th.: Solvatochromism of the $\pi^* \leftarrow n$ Transition of Acetone by Combined Quantum Mechanical–Classical Mechanical Calculations, 1067
Dorfman, S. See Fuks, D., 881, 897
Dupuis, M. See Aida, M., 949

Enchev, V.
Tautomerism in 2,2′-Bipyridyl-3/3′-diol, 721
Essuffar, M.
—; Luna, A.; Mó, O.; Yáñez, M.: High-Level Ab Initio Calculations on $CH_2^+(^2A_1) + PO(^2\Pi)$ Reactions, 559
Evleth, E. M. See Kozmutza, C., 775

Faegri Jr., K. See Swang, O., 105
Fang, D.-C.
—; Fu, X.-Y.: *Ab initio* Studies on the Mechanism of the Fluoroketene-imine Cycloaddition Reaction: Via a *gauche* or *trans* Intermediate, 1107
Fang, D.-C. See Fu, X.-Y., 715
Fares, M. See Bouferguene, A., 801
Ferenczy, G. G.
The Self Consistent Nonorthogonal Group-Function Approach in Reduced Basis Frozen-Core Calculations, 361
Fišer, J.
—; Vojtík, J.: CI Study of Rovibrational Dependence of Nuclear Quadrupole Coupling Constants of All Isotopic Variants of OH^+ in the $X^3\Sigma^-$ State, 441
Flamant, I.
—; Mosley, D. H.; Delhalle, J.; André, J. M.; Fripiat, J. G.: RHF Ab Initio Electronic and Molecular Structures of a $(-Be_2-)_\infty$ Chain, 871
Flock, M. See Cheng, V. K. W., 929
Fois, E. S. See Marx, D., 655
Fraija, F. See Bacchus-Montabonel, M. C., 611
Friedemann, R.
—; Breitkopf, C.: Theoretical Studies on the Decarboxylation Reaction in Thiamin Catalysis, 943
Fripiat, J. G. See Flamant, I., 871
Fu, X.-Y.
—; Li, Q.-M.; Fang, D.-C.: Theoretical Studies on the Elimination of Hydrogen Fluoride from Alkyl Fluoride and Its Substituent Effect, 715
Fu, X.-Y. See Fang, D.-C., 1107
Fuks, D.
—; Dorfman, S.: Effective Mixing Potentials and Ordering Thermodynamics of Alloys, 897
Fuks, D.
—; Dorfman, S.: Phase Diagram of Atom–Vacancy Solid Solution, 881

Galasso, V.
Theoretical Study of Spectroscopic Properties of Bicyclobutane, Tricyclopentane, Tricyclphexane, and Octabisvalene, 587
Gázquez, J. L.
—; Robles, J.: On the Conjoint Gradient Correction to the Hartree–Fock Kinetic and Exchange Energy Density Functionals, 3
Gianinetti, E.
—; Vandoni, I.; Colombo, S.: Optimization of a Spin-Coupled Wave Function Built with Partially Orthogonalized Orbitals, 369
González, J. See Suárez, D., 493
Grebneva, H. A. See Tolpygo, K. B., 219
Grigor'ev, A. I. See Rykova, E. A., 697
Gritsenko, O.
—; van Leeuwen, R.; Baerends, E. J.: Structure of the Opti-

mized Effective Kohn–Sham Exchange Potential and Its Gradient Approximations, 17
Gropen, O. See Swang, O., 105
Guenzburger, D. See Nogueira, S. R., 471

Halász, G. See Mayer, I., 1049
Hale, R. G. See Bishop, R. F., 919
Han, S. See Reinhardt, W. P., 327
Handy, N. C. See Altmann, J. A., 533
Hansen, A. E. See Kirby, R. A., 199
Hansen, T. B. See Avery, J., 401
He, Z.
—; Kraka, E.; Cremer, D.: Application of Quadratic CI with Singles, Doubles, and Triples (QCISDT): An Attractive Alternative to CCSDT, 157
Heitz, M.-C. See Daniel, C., 595
Herschbach, D. R.
Dimensional Scaling and Renormalization, 295
Ho, T.-M.
—; Chang, T.-C.: Electric-Field Gradient Calculations for Atoms with Axial Symmetry, 229
Hobza, P. See Šponer, J., 959
Hobza, P. See Vacek, J., 551
Hoggan, P. E. See Bouferguene, A., 801

Inaba, H. See Tachibana, A., 673
Ingamells, V. E. See Altmann, J. A., 533
Inokuti, M.
Remarks on Stopping Power: Its Connections with Particle Transport and with the Electronic Structure of Matter, 173

Jeung, G.-H. See Yiannopoulou, A., 575
Jursic, B. S.
Density Functional Calculations of Difluorodiazete Structures with Gaussian-Orbital-Type Approach, 213

Kaneko, M. See Aida, M., 949
Kapuy, E. See Kozmutza, C., 775
Kawauchi, S. See Tachibana, A., 673
Keith, T. A.
—; Bader, R. F. W.; Aray, Y.: Structural Homeomorphism Between the Electron Density and the Virial Field, 183
Khavryutchenko, D. See Sheka, F., 741
Kibler, M. See Negadi, T., 53
Kinghorn, D. B.
Integrals and Derivatives for Correlated Gaussian Functions Using Matrix Differential Calculus, 141
Kirby, R. A.
—; Hansen, A. E.: Study of Locally Dense and Locally Saturated Basis Sets in Localized Molecular Orbital Calculations of Nuclear Shielding: Ab Initio LORG Calculations for ^{13}C and ^{17}O in Norbornenone, 199
Klimenko, N. M. See Rykova, E. A., 697
Koga, T.
—; Thakkar, A. J.: Kinetic Energy Analysis of Atomic Multiplets, 89
Kolezynski, A. See Tkacz-Smiech, K., 1097
Kozmutza, C.
—; Kapuy, E.; Evleth, E. M.; Pipek, J.; Trézl, L.: Application of the Localized Representation for Studying Interaction Energies, 775
Kraka, E., See He, Z., 157
Krechl, J. See Cárdenas, R., 245
Kühn, O.
—; Malzahn, D.; May, V.: Theoretical Description of Dissipative Vibrational Dynamics Using the Density Matrix in the State Representation, 343
Kuntz, P. J. See Polák, R., 429
Kwiatkowski, T. See Olszewski, S., 113

La Manna, G.
—; Barone, G.: The Molecular Structure of *N*-Hydroxyurea, 971
La Manna, G. See Ramusino, M. C., 729
Légaré, P. See Mikušík, P., 887
Leininger, T. See Yiannopoulou, A., 575
Leszczynski, J. See Nowek, A., 757
Li, Q.-M. See Fu, X.-Y., 715
Li, Z.
—; Tao, F.-M.; Pan, Y.-K.: Calculation of Bond Dissociation Energies of Diatomic Molecules Using Bond Function Basis Sets with Counterpoise Corrections, 207
Lindgren, I.
Relativistic Many-Body and QED Calculations on Atomic Systems, 683
Liška, M. See Turi Nagy, L., 843
Lohr, L. L.
Energies and Structures of Rotating Argon Clusters: Analytic Descriptions and Numerical Simulations, 707
Longo, E. See Martins, J. B. L., 861
López, R. See Suárez, D., 493
Löwdin, P.-O.
In Memory of Jean-Louis Calais, 1
Luna, A. See Essuffar, M., 559
Lyyra, A. M. See Yiannopoulou, A., 575

Malzahn, D. See Kühn, O., 343
Manz, J. See Daniel, C., 595
Martins, J. B. L.
—; Andrés, J.; Longo, E.; Taft, C. A.: H_2O and H_2 Interaction with ZnO Surfaces: A MNDO, AM1, and PM3 Theoretical Study with Large Cluster Models, 861
Marx, D.
—; Fois, E. S.; Parrinello, M.: Static and Dynamic Density Functional Investigation of Hydrated Beryllium Dications, 655
Matsen, F. A.
Spin-Free Quantum Chemistry. XXVI. The Ising, Small-Bipolaron Theory of Cuprate Superconductivity, 1057
Mavri, J. See Berendsen, H. J. C., 975

May, V. See Kühn, O., 343
Mayer, I.
—; Vibók, Á.; Halász, G.; Valiron, P.: BSSE-Free SCF Algorithm for Intermolecular Interactions. III. Generalization for Three-Body Systems and for Using Bond Functions, 1049
Mella, M. See Bianchi, R., 321
Mikušík, P.
—; Pick, Š.; Castellani, N. J.; Légaré, P.; Demangeat, C.: Hydrogen Chemisorption on Pt/Ni(111) Systems, 887
Minaev, B. F.
—; Ågren, H.: Spin-Catalysis Phenomena, 519
Mizell Jr., J. R. See Morrison, R. C., 355
Mó, O. See Essuffar, M., 559
Morales, D. A.
Analytical Formulas for the Eigenvalues and Eigenfunctions of a *d*-Dimensional Hydrogen Atom with a Potential Defined by Gauss' Law, 7
Morosi, G. See Bianchi, R., 321
Morrison, R. C.
—; Mizell Jr., J. R.; Day Jr., O. W.: Generalized Overlap Amplitudes for the Lithium Atom, 355
Mosley, D. H. See Flamant, I., 871
Mrozek, J. See Nalewajski, R. F., 377
Musashi, Y. See Sakaki, S., 481

Nakamura, K. See Tachibana, A., 673
Nalewajski, R. F.
—; Mrozek, J.: Hartree–Fock Difference Approach to Chemical Valence: Three-Electron Indices in UHF Approximation, 377
Negadi, T.
—; Kibler, M.: The Periodic Table in Flatland, 53
Nogueira, S. R.
—; Guenzburger, D.: Relativistic Effects on the Electronic Structure and Bonding of $[Ir(CN)_5]^{3-}$, 471
Nowek, A.
—; Leszczynski, J.: An Ab Initio Study on HXC=O ··· HY Molecular Complexes (X, Y = F, Cl), 757
Núñez, M. A.
Asymptotic Behavior of Electron Densities and Computation of One-Electron Properties, 1077

Öhrn, Y. See Champagne, B., 811
Olszewski, S.
Distribution of Electron Orbits Having a Definite Angular Momentum in a Static Magnetic Field, 35
Olszewski, S.
—; Kwiatkowski, T.: Properties of Non-Bloch LCAO Wave Functions for Cubic Crystals in the Presence of an External Electric Field, 113
Ortí, E. See Rubio, M., 567

Paidarová, I. See Polák, R., 429
Pan, Y.-K. See Li, Z., 207
Park, J. K. See Seong, J., 79
Parrinello, M. See Marx, D., 655
Pavesi, L. See Bonapasta, A. A., 823
Perdew, J. P.
—; Burke, K.: Comparison Shopping for a Gradient-Corrected Density Functional, 309
Perez, J. J. see Alkorta, I., 123
Pick, Š. See Mikušík, P., 887
Pipek, J. See Kozmutza, C., 775
Polák, R.
—; Paidarová, I.; Špirko, V.; Kuntz, P. J.: On the Fragmentation Dynamics of $NH_3 \rightarrow NH_2 + H$. I. MRD CI Potential Energy Surfaces, 429
Ponec, R. See Cooper, D. L., 501
Ptak, W. S. See Tkacz-Smiech, K., 1097

Ramek, M. See Cheng, V. K. W., 929
Ramusino, M. C.
—; La Manna, G.: Ab Initio Study of Lithiated *N*-Methylpyridones, 729
Raos, G. See Cooper, D. L., 501
Reinhardt, W. P.
—; Han, S.: Exploiting the Analyticity of Schrödinger Operators: Theory and the Computation of Partial Cross Sections, 327
Repyakh, I.
First π-Electron Transitions in Finite Polymethine Chains, 913
Repyakh, I. V. See Andreev, Ye. A., 767
Requena, A. See Zúñiga, J., 43
Rivas-Silva, J. F. See Berrondo, M., 1115
Robles, J. See Gázquez, J. L., 3
Rubio, M.
—; Ortí, E.; Sánchez-Marín, J.: A Study of Coronene–Coronene Association Using Atom–Atom Pair Potentials, 567
Rutkowski, A. See Schwarz, W. H. E., 641
Rykova, E. A.
—; Klimenko, N. M.; Grigor'ev, A. I.: Theoretical Studies of Structure, Stability, and Chemical Bonding in Oxohydride OM_4H_6 Complexes, 697

Saalfrank, P. See Daniel, C., 595
Sakaki, S.
—; Musashi, Y.: A Theoretical Study on CO_2 Insertion into an M—H Bond (M = Rh and Cu), 481
Sánchez-Marín, J. See Rubio, M., 567
Schierbaum, K. D.
—; Xu, W.-X.: The Electronic Structure of Intrinsic Defects at TiO_2(110) Surfaces: An Ab Initio Molecular Orbital Study, 1121
Schwarz, W. H. E.
—; Rutkowski, A.; Wang, S. G.: Understanding Relativistic Effects of Chemical Bonding, 641
Seong, J.
—; Park, J. K.; Sun, H.: Ab Initio Study on NH^+: Transition Dipole Moments, Transition Probabilities, and Radiative Lifetimes, 79

Sheka, F.
—; Khavryutchenko, D.; Zayetz, A.: Computer Modeling of Assembly of Atoms in Electric Field, 741
Snijders, J. G. See van Lenthe, E., 281
Song, X. See Bu, Y., 95
Sordo, J. A. See Suárez, D., 493
Sordo, T. L. See Suárez, D., 493
Špirko, V. See Polák, R., 429
Šponer, J.
—; Hobza, P.: DNA Base Amino Groups and Their Role in Molecular Interactions: Ab Initio and Preliminary Density Functional Theory Calculations, 959
Starikov, E. B.
Ab Initio Crystal Orbital Calculations on Three-Dimensional Crystals of Large Bioorganic Molecules and Polymers, 851
Suárez, D.
—; López, R.; González, J.; Sordo, T. L.; Sordo, J. A.: Ab Initio Study of the Effect of CH ··· O Hydrogen Bonding on the *Exo/Endo* Stereoselectivity of Diels–Alder Reactions of 2-Substituted-1,3-Dienes with Sulfur Dioxide, 493
Sun, H. See Seong, J., 79
Swang, O.
—; Faegri Jr., K.; Gropen, O.; Wahlgren, U.: Chemisorption of Hydrogen and Oxygen Atoms on a Cobalt Surface: A Quantum Chemical Cluster Model Study, 105

Tachibana, A.
New Formulation of the Analytical Electronic Energy and the Regional Density Functional Theory, 423
Tachibana, A.
—; Kawauchi, S.; Nakamura, K.; Inaba, H.: Density Functional Theory of Chemical Reactivity Indices in Some Ion–Molecule Reaction Systems, 673
Taft, C. A. See Martins, J. B. L., 861
Tao, F.-M. See Li, Z., 207
Tapia, O. See Cárdenas, R., 245
Taşeli, H.
On the Exact Solution of the Schrödinger Equation with a Quartic Anharmonicity, 63
Tchougréeff, A. L.
Quantum Mechanical Models in Catalysis, 413
Tchougréeff, A. L.
—; Darkhovsky, M. B.: Lattice Relaxation and Order in the Low-Spin to High-Spin Transitions in Molecular Crystals, 903
Thakkar, A. J. See Koga, T., 89
Thorsteinsson, T. See Cooper, D. L., 501
Titov, A. V.
A Two-Step Method of Calculation of the Electronic Structure of Molecules with Heavy Atoms: Theoretical Aspect, 453
Tkacz-Smiech, K.
—; Ptak, W. S.; Kolezynski, A.: Model Potentials in Studies of Atomic Electron Density Distribution, 1097
Tolpygo, K. B.
—; Grebneva, H. A.: Effect of the State of *h-b*-1 Hydrogen Bond on the Character of Some Atom Vibrations in Guanine–Cytosine Pair of the DNA Molecule, 219
Trézl, L. See Kozmutza, C., 775
Trindle, C.
—; Datta, S. N.: Molecular Orbital Studies on the Spin States of Nitroxide Species: Bis- and Trisnitroxymetaphenylene, 1,1-bis nitroxyphenylethylene, and 4,6-Dimethoxy-1,3-dialkylnitroxybenzenes, 781
Tunega, D. See Turi Nagy, L., 843
Turi Nagy, L.
—; Tunega, D.; Liška, M.: Modeling of Interaction Properties of Surfaces of Phyllosilicates: A Theoretical Forecast of Adsorption Isotherms of Noble Gases at the Talc Surface, 843

Vacek, J.
—; Hobza, P.: On the Thermodynamic Character of the Benzene ··· Ar_2 Complex: An Application of the Ab Initio Intermolecular Potential, 551
Valiron, P. See Mayer, I., 1049
Vandoni, I. See Gianinetti, E., 369
van Duijnen, P. Th. See de Vries, A. H., 1067
van Leeuwen, R. See Gritsenko, O., 17
van Leeuwen, R. See van Lenthe, E., 281
van Lenthe, E.
—; van Leeuwen, R.; Baerends, E. J.; Snijders, J. G.: Relativistic Regular Two-Component Hamiltonians, 281
Vibók, Á. See Mayer, I., 1049
Vivie-Riedle, R. De. See Daniel, C., 595
Vojtík, J.
Static Characteristics of the Ionization Event in the He(2^3S)2HD Collision System, 545
Vojtík, J. See Fišer, J., 441

Wahlgren, U. See Swang, O., 105
Wang, B.-C.
—; Yu, L.-J.; Wang, W.-J.: A Semiempirical Study of $C_{24}N_4$ and Its Boron–Nitrogen Analogs, 465
Wang, M. See Avery, J., 401
Wang, S. G. See Schwarz, W. H. E., 641
Wang, W.-J. See Wang, B.-C., 465
Wasilewski, J.
A Classification of Open-Shell States of Molecules, 625
Weniger, E. J.
Nonlinear Sequence Transformations: A Computational Tool for Quantum Mechanical and Quantum Chemical Calculations, 265
Whaley, K. B.
—; *Review of Quantum Mechanics in Chemistry*, by G. C. Schatz and M. A. Ratner, 1131

Xian, Y. See Bishop, R. F., 919
Xu, W.-X. See Schierbaum, K. D., 1121

Yamabe, T. See Yamaguchi, Y., 73
Yamaguchi, Y.
—; Yamabe, T.: Ab Initio Torsional Potentials in Silole Dimers, 73
Yáñez, M. See Essuffar, M., 559
Yiannopoulou, A.
—; Leininger, T.; Lyyra, A. M.; Jeung, G.-H.: Theoretically Calculated Rovibronic Transition Spectra of KRb, 575
Yu, L.-J. See Wang, B.-C., 465
Zayetz, A. See Sheka, F., 741
Zúñiga, J.
—; Alacid, M.; Requena, A.; Bastida, A.: Matrix Elements for the Modified Pöschl–Teller Potential, 43

International Journal of Quantum Chemistry Subject Index—Volume 57

α, α elimination, 715
α, β elimination, 715
Ab initio, 1107, 1115
Ab initio (4-31G basis set) method, 721
Ab initio calculations, 199, 493, 559, 575, 697, 729, 959, 971
Ab initio crystal orbital calculations, 851
Ab initio dynamic polarizabilities, 811
Ab initio effective valence-shell Hamiltonian (H^v) method, 79
Ab initio intermolecular potential, 551
Ab initio molecular orbital calculations, 673
Ab initio molecular orbital method, 73
Ab initio self-consistent field (SCF), 929, 949
Ab initio self-consistent-field (SCF) cluster approach, 1121
Ab inition configuration interaction methods, 611
Ab initio SCF and spin-coupled wave functions, 501
Adsorption isotherms, 843
Aggregated oxygen vacancies, 1121
All-electron calculations, 105
Alloys, 897
AM1, 861
Analytical electronic energy, 423
Analyticity, 327
Ancillary H-Bonding Molecules, 245
Angular momentum, 35
Anharmonic vibrational states, 95
Anti-conformation, 73
Argon clusters, 707
Aromatic ring, 729
Atom–atom pair potential, 567
Atomic electric-field gradient (EFG), 229
Atomic multiplet states, 89
Atomic partial photoionization cross sections, 327
Atoms, 741
Atom–vacancy solid solution, 881
Atom vibrations, 219
Axial symmetry, 229
Aziz pair potential, 707

Band gaps, 1115
Basis sets, 533
Becke's gradient correction, 655
Benzene $\cdots$ Ar_2 cluster, 551
Beryllium clusters, 871
Bohr–Sommerfeld quantization rules, 35
Bond function basis sets, 207
Born–Oppenheimer approximations, 625
Boron ions, 611
Boron–nitrogen analogs, 465
Breit interactions, 683
BSSE-free SCF method, 1049

Car–Parrinello method, 655
Catalytic processes, 413
CCSDT, 157
CH $\cdots$ O electrostatic interaction, 493
CHA/E formalism, 1049
Chemical bonding, 471, 697
Chemisorption, 105
Closed-form eigenfunctions, 63
Cluster–adsorbate bonding energy, 105
Cluster models, 1115
Cluster stability, 767
CNDO/2, 767
CO_2 Insertion, 481
Collisions, 611
Computer modeling, 741
Configuration interaction (CI), 441
Constant energy molecular dynamics simulations, 551
Coronene–coronene association, 567
Correlated Gaussian functions, 141
Counterpoise procedure, 207
Coupled-cluster method (CCM), 919
Coupled Hatree–Fock level of approximation, 811
Crystals, 851
Cubic crystals, 113
Cubic valence numbers, 377
Cuprate superconductivity, 1057
Cyclic polyene rings, 1019

Dahne's triad theory, 913
d-dependent potential, 7
D-dimensional Coulomb system, 53
d-dimensional hydrogen atom, 7
Deep point defects, 823
Defect interaction parameters, 881
Density functional calculations, 105
Density functional theory (DFT), 309, 423, 471, 533, 655, 673, 1097
Density functional theory (DFT) calculations, 959
Density functional theory (DFT) methods, 213
Density matrix evolution (DME) method, 975
Dielectric continuum, 1067
Diels–Alder reactions, 493
Differential operators, 43
Dimensional scaling, 295
Dirac Hamiltonian, 281
Dissipative dynamics, 343
Dissociation dynamics, 429
DNA base amino groups, 959
Double-zeta atomic basis sets, 811
Dynamical correlation effects, 587

Effective core potential (ECP) method, 453
Effective potential approach, 897
Effective valencies, 501
Eigenfunctions, 391
Eigenvalues, 235
Electric field, 741

Electron capture processes, 611
Electron densities, 1077
Electronic band gap states, 1121
Electronic configurations, 625
Electronic structure, 471
Electronic structure of matter, 173
Electronic structures, 1121
Electron orbits, 35
Electron transfer (ET), 673
Electron transitions, 113
Equations-of-motions (EOM), 587
Exact theorems, 641
Exchange-correlation energy, 309
Exchange energy functionals, 3
exo/endo stereoselectivity, 493
Explicit, polarizable molecular solvent models, 1067
Extended Koopman's theorem (EKT), 391
External electric field, 113

Feynman–Dyson amplitudes, 355
Finite chains, 871
Finite energy gap, 913
Flatland ($D = 2$), 53
Force-field version PIMM90, 943
Fourth-order Møller–Plesset approximation (MP4), 207
Full geometry optimizations, 757

G2 theory, 559
Gas–solid interaction potential, 843
Gauche intermediate, 1107
Gauss' law, 7
Gaussian basis sets, 533
Generalized gradient expansion approximation, 3
Generalized overlap amplitudes (GOAS), 355, 391
Gold clusters, 735
Gradient approximations, 17
Gradient corrections, 309
Guanine–cytosine (G–C) pair, 219

H_2O and H_2 interaction, 861
Hamiltonians, 281
Harmonic oscillator, 63
Harmonic vibrational frequencies, 655
Hartree–Fock approximation, 3
Hartree–Fock methods, 533
Hartree–Fock–Slater–Pauli calculations, 641
Hartree–Fock theory, 281
Hartree–Fock (UHF) approximation, 377
He(2^3S)2HD collision system, 543
Heavy atoms, 453
Hessian eigenvalues, 567
Heterofullerenes, 465
Highest occupied molecular orbital (HOMO), 949
High spin states, 781
High-spin transitions, 903
Hilbert spaces, 1077
Hydride-transfer step, liver alcohol dehydrogenase, 245
Hydrogen abstraction (HA), 673
Hydrogen atom transfer, 95
Hydrogen bond, 219
Hydrogen chains, 811
Hydrogen chemisorption, 887
Hydrogen interaction, in GaAs, 823
Hyperbolic functions, 43

Infrared (IR) lasers, 595
Integral formulas, 141
Interaction energy, 775
Interaction potentials, 567
Internal rotation, 73
Interpolant Polynomial Technique, 1019, 1033
Intramolecular hydrogen bond, 971
Intramolecular hydrogen bonding, 943
Intramolecular interactions, 929
Intrinsic reaction coordinate (IRC), 673
Ionic Crystals, 1115
Ionization event, 543
Ising, small-bipolaran theory, 1057
Isoelectronic reactions, 673
Isolated oxygen vacancies, 1121
Isotopic variants, 441

Kinetic energy analysis, 89
Kinetic energy functionals, 3
Kohn–Sham exchange potential, 17
Kohn–Sham scheme, 1097

Lamb-shift calculations, 683
Large cluster models, 861
Lattice spin models, 235
Least-motion maximum-overlap mechanism, 943
Least-squares fitting, 321
Lennard-Jones oscillator (LJO) pair potentials, 707
Lieb conjecture, 449
Lithium atom, 355
Localized many-body perturbation theory (LMBPT), 775
Localized orbital/local origin (LORG) approach, 199
Locally dense sets, 199
Locally saturated sets, 199
Local spin density (LSD) approximation, 309
Logarithmic potential energy function, 7
Low-spin transitions, 903
Lower bound, 449

M—H bond energy, 481
Madelung rule, 53
Many-body effects, 295
Many-body perturbation methods, 683
Many-center Coulomb potentials, 401
Many-electron atomic system, 1097
Many-electron wave functions, 413
Matrix differential calculus, 141
Matrix elements, 43, 113
Metal core-level shifts, 887
Metal–ligand bonds, 595
Minimum-energy structures, 971
MNDO, 861
MNDO–PM3 method, 721
Model transition structure, (TS), 245
Molecular complexes, 757
Molecular crystals, 903
Molecular dissociation energies, 207
Molecular dynamics (MD) simulation, 975
Molecular electrostatic potential (MEP), 123
Molecular open-shell states, 625
Molecular orbital (MO) study, 735, 781
Molecular polarization potential maps (MPP), 123
Momentum space, 401
Morse potentials, 79

MRD–CI extrapolation, 429
Multicenter electronic integrals, 801

Noble gases, 843
Nonadiabatic transitions, 975
Non-Bloch LCAO wave functions, 113
Nonempirical pair potential, 897
Nonorthogonal formalism, 361
Nonrelativistic approximations, 625
Normalized advance coordinate (NAC), 245
Nuclear quadrupole coupling constants, 441
Nuclear shielding, 199
Nucleic acid bases, 123
Numerical basis sets, 533

One-center two-range expansion method, 801
One-dimensional chain, 919
One-dimensional Hubbard model, 1019, 1033
One-electron effective core potential, 105
One-electron properties, 1077
Optimized potential model (OPM), 17
Orbitals, 369, 453
Organometallics, 595
Orthogonal group function approach, 361
Orthogonalized atomic orbitals (OAO), 377
Outer-valence Green function (OVGF), 587
Oxohydride OM_4H_6 complexes, 697

π-electron transitions energies, 913
Pair populations, 501
Paramagnetic catalyst, 519
Pariser–Parr–Pople method, 913
Pariser–Parr–Pople (PPP) model, 1019, 1033
Partially orthogonalized orbitals, 369
Particle-transport theory, 173
Pauli Hamiltonian, 281
Penning processes, 543
Periodic table, 53
Perturbation expansion, 281
Perturbation theory, 641
Photodesorption, 595
Planar conjugated systems, 781
Platinum 5*d* orbitals, 735
PM3, 861
Pöschl–Teller potential, 43
Post-Hartree–Fock calculations, 747
Potential energy curves, 575
Potential energy density, 183
Potential energy surface (PES), 429
Potential energy surfaces (PES), 929
Proton transfer (PT), 673, 975
Puckering, 949

QCISDT, 157
Quantum-electrodynamics (QED), 683
Quantum mechanical–classical mechanical approach, 1067
Quantum Monte Carlo methods, 321
Quantum-phase transitions, 919
Quartic Anharmonicity, 63

Radiative lifetimes, 79
Random-phase approximation, 811
Random-phase approximation (RPA), 587
Rayleigh–Schrödinger perturbation series, 265
Reciprocal-space Schrödinger equation, 401
Reduced basis frozen-core calculations, 361
Reduced statistical density operator, 343
Regularized two-component relativistic Hamiltonians, 281
Relativistic effects, 471
Relativistic molecular virial theorem, 641
Remainder estimates, 265
Renormalization, 295
Restricted Hartree–Fock calculations, 89
RHF ab initio electronic structures, 871
RHF ab initio models, 213
RHF ab initio molecular structures, 871
RKR potentials, 79
Rotating argon clusters, 707
Rovibrational dependence, 441

6-31G* basis set, 729
6-31G** basis set, 715
Schrödinger equation, 7, 63, 321
Schrödinger operators, 327
Schrödinger stress tensor, 183
Secular matrices, 235
Secular polynomials, 235
Semiempirical AM1 method, 721
Semiempirical AM1 methods, 943
Semiempirical PM3 methods, 943
Separated atoms limit (SAL), 377
Sequence transformations, 265
Ser-48, 245
Shallow impurities, 823
Silole dimers, 73
Singlet potential energy surfaces, 559
Singlet–singlet transitions, 575
Size-extensive quadratic CI method, 157
Slater-type orbital package (STOP), 801
Spherical symmetric constraint, 229
Spin-$\frac{1}{2}$ anisotropic Heisenberg models, 919
Spin-catalysis, 519
Spin-coupled wave function, 369
Spin coupling, 781
Spin models, 919
Spin-prohibition, 519
Spin transitions, 903
Static concentration wave (SCW) theory, 897
Static magnetic field, 35
Sternheimer's core polarization effect, 229
STO-3G basis sets, 811
Stopping power, 173
Structural homeomorphism, 183
Sturmian basis sets, 401
Surface–atom local density of electronic-state properties, 887
Surface reacitivity, 887

Talc, 843
Tautomerism, 721
T correlation effects, 157
Thermal energy collisions, 543
Thermodynamics, 897

Thiamin systems, 943
Thomas–Fermi kinetic energy, 449
Three-component systems, 1049
Three-dimensional crystals, 851
Thymine dimer radical cation, 949
Time-dependent perturbation theory expression, 95
Trans intermediate, 1107
Transition dipole moments, 575
Transition electric dipole moments, 79
Transition-metal complexes, 903
Transition Probabilities, 79
Transition state (TS), 481
Triplet potential energy surfaces, 559
Triplet–triplet transitions, 575
Tunneling, 95
Two-dimensional square lattice, 919
Two-electron systems, 449

Ultraviolet (UV) lasers, 595

Vacancy-type defects (VTD), 881
Vanderbilt's ultrasoft pseudopotentials, 655
Vibrational dynamics, 343
Vibrational frequency calculations, 757
Vibrational mediated photodissociation, 595
Vibrational population factors, 543
Virial field $\mathscr{V}(\mathbf{r})$, 183

Water dissociation, 767
Water fractals, 767
Wave-function optimization, 321